Surface Vision Transformers: Attention-Based Modelling applied to Cortical Analysis

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Abstract

The extension of convolutional neural networks (CNNs) to non-Euclidean geometries has led to multiple frameworks for studying manifolds. Many of those methods have shown design limitations resulting in poor modelling of long-range associations, as the generalisation of convolutions to irregular surfaces is non-trivial. Motivated by the success of attention-modelling in computer vision, we translate convolution-free vision transformer approaches to surface data, to introduce a domain-agnostic architecture to study any surface data projected onto a spherical manifold. Here, surface patching is achieved by representing spherical data as a sequence of triangular patches, extracted from a subdivided icosphere. A transformer model encodes the sequence of patches via successive multi-head self-attention layers while preserving the sequence resolution. We validate the performance of the proposed Surface Vision Transformer (SiT) on the task of phenotype regression from cortical surface metrics derived from the Developing Human Connectome Project (dHCP). Experiments show that the SiT generally outperforms surface CNNs, while performing comparably on registered and unregistered data. Analysis of transformer attention maps offers strong potential to characterise subtle cognitive developmental patterns.

Keywords: Vision Transformer, Cortical Analysis, Deep Learning, Neuroimaging, Attention-based Modelling.
1. Introduction

Over recent years, attention-based transformer models have dominated the field of natural language processing (NLP) through supporting the learning of long-distance associations within sequences (Vaswani et al., 2017; Radford et al., 2018; Devlin et al., 2019). Since thorough understanding of context within images is essential for most computer vision task, Dosovitskiy et al. 2020 proposed the vision transformer (ViT) to adapt NLP transformer architectures (Vaswani et al., 2017) to the natural imaging domain, by processing images as sequences of patches. In doing so, they showed that pure transformer models were capable of outperforming CNNs for image classification, while addressing some of their limitations in terms of their inductive bias towards local features, lack of scalability and low parameter-efficiency.

As there is no generic deep learning method for studying non-Euclidean data, there has also been an emerging interest in translating attention-based mechanisms to irregular geometries, as a way to improve the learning of long-range associations and feature expressiveness. The transformer architecture has been used with some successes in graph domain (Yang et al., 2021; Dwivedi and Bresson, 2021), or for sequences of 3D meshes and point-clouds (Sarasua et al., 2021; Zhao et al., 2021; Guo et al., 2021), while He et al. 2021 introduced a self-attention mechanism for general manifolds to ensure gauge equivariance. However, to date, there has been no application of vision transformers to generic functions on surfaces, which are an important data structure across many distinct disciplines (Boomsma and Frellsen, 2017; Jiang et al., 2019; Defferrard et al., 2020), particularly in medical imaging (Gopinath et al., 2019; Kong and Shadden, 2021; Ma et al., 2021; Lebrat et al., 2021).

In this paper, we therefore seek to adapt the data efficient image transformer (DeiT) model (Touvron et al., 2020) to surface domains by projecting data onto a sphere and patching surfaces using a regular icospheric tessellation. The methodology of surface patching is general and the proposed SiT may be adapted for any genus-zero surface. One challenging area, which stands to particularly benefit from this style of analysis is the study of the cerebral cortex, since traditional approaches for brain image analysis based on registration, have historically been unable to fully capture the heterogeneity of cortical organisation across individuals, not only for vulnerable groups (Ciarrusta et al., 2020), but also within healthy populations (Fischl et al., 2008; Frost and Goebel, 2012; Glasser et al., 2016; Kong et al., 2019). We therefore evaluate our approach by comparing our model against a range of convolutional geometric deep learning frameworks on the task of developmental phenotype regression from cortical metric data derived from the Developing Human Connectome Project (dHCP).\footnote{The code is available at \url{https://github.com/metrics-lab/surface-vision-transformers}}

The main contributions of this work can be summarised as follows:

- This paper proposes translation of vision transformers (Dosovitskiy et al., 2020; Touvron et al., 2020) to any data associated with genus-zero surfaces.

- Validation of the model on the task of neurodevelopmental phenotype regression demonstrates competitive performance relative to spectral and spatial geometric deep learning frameworks (Cohen et al., 2018; Monti et al., 2016; Defferrard et al., 2017; Kipf and Welling, 2017; Zhao et al., 2019).
Visualisation of attention weights highlights that the model attends to well-characterised spatiotemporal patterns of perinatal cortical development (Dubois et al., 2008; Doria et al., 2010; Eyre et al., 2021).

2. Related work

Attention-based modelling and Transformers. Attention was first introduced by Bahdanau et al. 2016 as a tool for modelling long-range dependencies, in recurrent networks trained for machine translation tasks. To increase context modelling in long-sequences, Vaswani et al. 2017 introduced the self-attention mechanism - learning attention between elements in a sequence - with the transformer architecture. When paired with pre-training on very large datasets, this led to powerful language models such as BERT or GPT (Devlin et al., 2019; Radford et al., 2018), that are transferable to many downstream tasks. While CNNs have proven to be sample-efficient architectures for image understanding, most architectures saturate in performance when presented with very large datasets, and struggle to relate distant elements within images. This is partly due to the inherent inductive biases (locality and translational equivariance) of the CNN architecture. As a result, inspired by the success of attention mechanisms, efforts have been made to incorporate attention-based operations into CNNs (Jaderberg et al., 2016; Wang et al., 2018a; Hu et al., 2019), including for medical imaging (Wang et al., 2018b; Schlemper et al., 2019), as a way to increase the learning of contextual information. However, these have been limited by the heavy cost of pixel-level attention and so computation was mostly restricted to low-resolution feature maps. More recently, vision transformer architectures have been introduced to adapt the sequence-modelling of NLP in the context of computer vision. Dosovitskiy et al. 2020 introduced a patching strategy consisting of splitting RGB images into patches of shape $16 \times 16 \times 3$. By doing so, the attention is computed at the patch level, and contextual information from the entire image is available already from early layers. These have been shown to outperform CNNs for a range of computer vision tasks including image classification and segmentation (Dosovitskiy et al., 2020; Touvron et al., 2020; d’Ascoli et al., 2021), object detection (Xu et al., 2021) and video classification (Liu et al., 2021), achieving state-of-the-art performance without relying on strong spatial priors. In medical imaging tasks, modelling long-range dependencies is critical, for instance for anomaly detection or image segmentation, but limited by most of the current convolution-based models. Therefore, hybrid and pure vision transformers have also been translated with success for medical image segmentation (Pinaya et al., 2021; Chen et al., 2021a; Karimi et al., 2021; Zhang et al., 2021a; Gao et al., 2021), medical image registration (Chen et al., 2021b; Zhang et al., 2021b; van Tulder et al., 2021) or medical image reconstruction (Feng et al., 2021).

Geometric Deep Learning. A prominent approach for studying cortical surfaces relies on geometric deep learning (gDL) methods (Gopinath et al., 2019; Arya et al., 2020; Kim et al., 2021) that aim to adapt Euclidean CNNs to irregular manifolds (Bronstein et al., 2016, 2021). While many frameworks for surface and graph convolutions exist, typically these frameworks struggle to learn rotationally equivariant, expressive features, without prohibitively high computational cost (Bruna et al., 2013; Cohen et al., 2018). These limitations have been stressed in a recent benchmarking paper (Fawaz et al., 2021), which evaluated geometric deep learning techniques in the context of cortical analysis.
3. Methods

3.1. Data

Data in this work comes from the publicly available third release of the Developing Human Connectome Project (dHCP)\(^2\) (Hughes et al., 2017) and contains cortical surface meshes and metrics (sulcal depth, curvature, cortical thickness and T1w/T2w myelination) derived from T1 and T2-weighted magnetic resonance images (MRI), processed according to Makropoulos et al. 2018 and references therein (Kuklisova-Murgasova et al., 2012; Schuh et al., 2017; Hughes et al., 2017; Cordero-Grande et al., 2018; Makropoulos et al., 2018). We included a total of 588 images acquired from term (born ≥ 37 weeks gestational age, GA) and preterm (< 37 weeks GA) neonatal subjects, scanned between 24 and 45 weeks postmenstrual age (PMA). Some of the preterm neonates were scanned twice: once after birth and again around term-equivalent age.

![Surface Vision Transformer (SiT) architecture](https://example.com/surface_vision_transformer.png)

Figure 1: Surface Vision Transformer (SiT) architecture. The cortical data is first resampled, using barycentric interpolation, from its template resolution (32492 vertices) to a sixth order icosphere (mesh of 40962 equally spaced vertices). The regular icosphere is divided into triangular patches of equal vertex count (b, c) that fully cover the sphere (not shown), which are flattened into feature vectors (d), and then fed into the transformer model.

The proposed framework was benchmarked on two phenotype regression tasks: prediction of postmenstrual age (PMA) at scan, and gestational age (GA) at birth. Since the objective is to model PMA and GA as markers of healthy development, all preterms’ second scans were excluded from the PMA prediction task, and their first scans were excluded from the GA regression task. This resulted in 530 neonatal subjects for the PMA prediction task (419 term/111 preterm), and 514 neonatal subjects (419 term/95 preterm) for the GA regression task.

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\(^2\) [http://www.developingconnectome.org](http://www.developingconnectome.org)
| Models   | Layers | Heads | Hidden size $D$ | MLP size | Params. |
|----------|--------|-------|----------------|----------|---------|
| SiT-tiny | 12     | 3     | 192            | 768      | 5M      |
| SiT-small| 12     | 6     | 384            | 1536     | 22M     |
| SiT-base | 12     | 12    | 768            | 3072     | 86M     |

Table 1: All SiT models preserve a hidden size of 64 per attention head.

prediction task. In all instances, the proposed transformer networks are compared against the best performing surface CNNs reported in Fawaz et al. 2021: Spherical UNet (Zhao et al., 2019), MoNet (Monti et al., 2016), GConvNet (Kipf and Welling, 2017), ChebNet (Defferrard et al., 2017) and S2CNN (Cohen et al., 2018); on cortical surface data following the same pre-processing pipeline as in Fawaz et al. 2021. Therefore, experiments were run on both template-aligned data and non-registered (native) data, and train/test/validation splits parallel those used in Fawaz et al. 2021. See Appendix A.3 for more details on image preprocessing and registration pipelines, and Appendix A.4 for training details of gDL methods.

3.2. Surface Vision Transformer

Architecture. The proposed SiT model builds upon three variants of the data efficient image transformer or DeiT (Touvron et al., 2020): DeiT-Tiny, DeiT-Small, DeiT-Base. For more details about the SiT model architectures see Table 1. In general terms, for any vision transformer, the high-resolution grid of the input domain $X$, is reshaped into a sequence of $N$ flattened patches $\tilde{X} = [\tilde{X}_1^{(0)}, ..., \tilde{X}_N^{(0)}] \in \mathbb{R}^{N \times (VC)}$ ($V$ vertices, $C$ channels). This initial sequence is first projected onto a sequence of dimension $D$ with a trainable linear layer; an extra token for regression is concatenated to the patch sequence, then a positional embedding is added to the patch embeddings, such that the input sequence of the transformer is $X^{(0)} = [X_0^{(0)}, ..., X_N^{(0)}] \in \mathbb{R}^{(N+1) \times D}$ (see details in Appendix C.2). For the SiT, this is implemented by imposing a low-resolution triangulated grid, on the input mesh, using a regularly tessellated icosphere (Fig 1). This generates 320 patches, per hemisphere, and per channel. In all cases, before extracting patches, the right hemisphere is flipped to mirror the left orientation. Since there are four input channels (myelin, sulcal depth, curvature and cortical thickness) and the number vertices per patch is 153, the total dimension per patch is $VC = 612$. The architecture is made of $L$ transformer blocks, each composed of a multi-head self-attention layer (MSA), implementing the self-attention mechanism across the sequence, and a feed-forward network (FFN), which expands then reduces the sequence dimension (see details in Appendix C.1). In short, for every transformer block at layer $l$, the input sequence $X^{(l)} = [X_0^{(l)}, ..., X_N^{(l)}]$ is processed as follows:

$$Z^{(l)} = MSA(X^{(l)}) + X^{(l)}$$
$$X^{(l+1)} = FFN(Z^{(l)}) + Z^{(l)}$$

Following standard practice in transformers, LayerNorm (Ba et al., 2016) is used prior to each MSA and FFN layer (omitted for clarity in Eq 1) and residual connections are
added thereafter. The MSA used in transformers runs multiple self-attention in parallel at each layer, referred as *Heads* in Table 1. In practice, it means that the input sequence of dimension $D$ is divided into sub-parts of dimension $D_h = D/h$. After being run in parallel, the self-attention heads are concatenated. The regression patch of the final sequence $X^{(L)}$ is used as input of an MLP head for prediction (see Fig 1).

**Attention maps.** Unlike CNNs, the vision transformer model learns associations between patches within a sequence thanks to a self-attention mechanism inherited from NLP Transformer (Vaswani et al., 2017). Attention maps can be visualised on the input space by propagating the attention weights across layers and heads from the regression token of the last transformer block (details in Appendix C.3). As each transformer head is running in parallel, they should attend to different parts of the input sequence.

**Pre-training.** Previous works pointed the necessity to pre-train vision transformers on large-scale datasets to mitigate the lack of inductive biases in the architecture (Dosovitskiy et al., 2020; Steiner et al., 2021; Beal et al., 2021). Lately, the need for large pretraining has been reviewed as alternative training strategies such as Knowledge Distillation have emerged (Touvron et al., 2020). This is relevant for medical imaging tasks, as datasets are usually smaller than in natural imaging, and can benefit from pretraining before transferring to downstream tasks. Therefore, in this paper we evaluate different training strategies, to explore: 1) training from scratch; 2) initialising from ImageNet weights (to support training on small datasets through incorporation of some spatial priors) and 3) fine-tuning after a self-supervision learning pretraining task (SSL). For ImageNet, we used pretrained models from the **timm** open-source library\(^3\), where models were pretrained on ImageNet2012 (1 million images, 1000 classes) on patches of size $16 \times 16 \times 3$. For self-supervision, we adapted the *masked patch prediction* task (MPP) for self-supervision used in BERT (Devlin et al., 2019), which consists of corrupting at random some input patches in the sequence; then training the network to learn how to reconstruct the full corrupted patches. In this setting, we corrupt at random 50% of the input patches, either replacing them with a learnable mask token (80%), another patch embedding from the sequence at random (10%) or keeping their original embeddings (10%). To optimise the reconstruction, the mean square error (MSE) loss is computed only for the patches in the sequence that were masked. Pretraining was performed with template (registered) training data only, as adding unregistered data to the pre-training did not seem to improve results (see Appendix B.1).

4. Results & Discussion

Test results for the tasks of postmenstrual age (PMA) at scan and gestational age (GA) at birth are reported in Table 2 for the three training strategies: training from scratch, from ImageNet weights and from SSL weights and compared against best gDL methods in Fawaz et al. 2021. Overall SiT models consistently outperformed two of the gDL methods (ChebNet and GConvNet) and were competitive compared to the three best performing geometric models (S2CNN, Spherical UNet and MoNet). Spherical UNet obtained excellent performances on template space for both tasks in Fawaz et al. 2021, but greatly underperformed on native space, since it builds no transformation equivariance into its model. **All SiT**

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3. pretrained models on ImageNet available at http://github.com/rwightman/pytorch-image-models/
models achieved similar performance to Spherical UNet on template, with improvements on PMA (0.55 for SiT-small), but dropped less in performance between template/native predictions: for instance SiT-tiny achieved 0.58/0.64 on PMA against 0.57/0.87 for Spherical UNet. This seems to indicate some robustness to transformation. Generally, SiT-tiny and SiT-small performed fairly well and consistently on both tasks, especially on finetuned models following self-supervision. Results would suggest the need of regularisation for SiT-base (especially dropout) whereas SiT-small achieved the best performance on average (template & native) for both tasks. Overall, almost all configurations of SiT achieved better average performances (on both tasks) than gDL methods, that were optimised with various data augmentation techniques in Fawaz et al. 2021.

Birth age task. The task of GA prediction is arguably more complicated than the PMA task, as it is run on scans acquired around term-equivalent age (≥ 37 weeks GA) for both term and preterm neonates, and therefore is highly correlated to PMA at scan. Therefore, a deconfounding strategy of PMA at scan for the task of birth age prediction was employed and described in details in Appendix B.2. SiT models achieved good performances without major drops in performance between template and native for this task, a trend that can be seen across SiT versions. For details of deconfounding of gDL methods see Appendix A.4.

Training methods. For the task of PMA at scan, while comparing the three training strategies, training from ImageNet often underperformed training from scratch, while training after the MPP task achieved the best performance with SiT-tiny and SiT-small. Self-supervision pretraining appeared to improve training quality, for nearly all configurations and both tasks. This is consistent with results in natural imaging. As a vision transformer is a more general (less inductive biases) architecture than a CNN, it seems natural that pretraining is beneficial to compensate for the lack of geometric prior.
Attention Maps. Figure 2 shows the attention per head for a preterm-born neonate (born at 26.7 weeks) that was scanned twice: once at 32.4 weeks and a second time at 41.9 weeks. Attention maps captured the well-characterised spatio-temporal patterns of perinatal brain development. Maturation of cortical regions follows a primary-to-association trajectory (Doria et al., 2010; Eyre et al., 2021), highlighted by increases in T1w/T2w myelin contrast in the visual, auditory and somatosensory areas, as well as rapid cortical folding over the third trimester, particularly in the parietal and frontal lobes (Dubois et al., 2008).

5. Conclusion

In this paper we translated the methodology of vision transformers to surfaces and validated on the challenging task of phenotype prediction from cortical imaging data. Vision transformers offer strong potential for analysing signals, such as cortical or cardiac, on surface, as they show robustness to transformations and can integrate information between distant regions. Future work could focus on improving training strategies, as the largest SiT architectures suffer from the limited size of medical datasets and could benefit from data augmentation, regularisation and alternative self-supervision pretraining strategies (Touvron et al., 2019; Kolesnikov et al., 2019).
Acknowledgments

We would like to acknowledge funding from the EPSRC Centre for Doctoral Training in Smart Medical Imaging (EP/S022104/1). Data were provided by the developing Human Connectome Project, KCL-Imperial-Oxford Consortium funded by the European Research Council under the European Union Seventh Framework Programme (FP/2007-2013) / ERC Grant Agreement no. [319456]. We are grateful to the families who generously supported this trial. CY/TSC/MFG were supported by NIH R01 MH060974.

References

Devanshu Arya, Richard Olij, Deepak K. Gupta, Ahmed El Gazzar, Guido van Wingen, Marcel Worry, and Rajat Mani Thomas. Fusing structural and functional {mri}s using graph convolutional networks for autism classification. In Medical Imaging with Deep Learning, 2020. URL https://openreview.net/forum?id=o07NxLQDYa.

Jimmy Lei Ba, Jamie Ryan Kiros, and Geoffrey E. Hinton. Layer normalization, 2016.

Dzmitry Bahdanau, Kyunghyun Cho, and Yoshua Bengio. Neural machine translation by jointly learning to align and translate, 2016.

Josh Beal, Hao-Yu Wu, Dong Huk Park, Andrew Zhai, and Dmitry Kislyuk. Billion-scale pretraining with vision transformers for multi-task visual representations. CoRR, abs/2108.05887, 2021. URL https://arxiv.org/abs/2108.05887.

Wouter Boomsma and Jes Frellsen. Spherical convolutions and their application in molecular modelling. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 30. Curran Associates, Inc., 2017. URL https://proceedings.neurips.cc/paper/2017/file/1113d7a766f0ceca1bb350bfe145467c6-Paper.pdf.

Jelena Bozek, Antonios Makropoulos, Andreas Schuh, Sean Fitzgibbon, Robert Wright, Matthew F. Glasser, Timothy S. Coalsen, Jonathan O’Muircheartaigh, Jana Hutter, Anthony N. Price, Lucilio Cordero-Grande, Rui Pedro A.G. Teixeira, Emer Hughes, Nora Tusor, Kelly Pegoretti Baruteau, Mary A. Rutherford, A. David Edwards, Joseph V. Hajnal, Stephen M. Smith, Daniel Rueckert, Mark Jenkinson, and Emma C. Robinson. Construction of a neonatal cortical surface atlas using multimodal surface matching in the developing human connectome project. NeuroImage, 179:11–29, 10 2018. ISSN 1095-9572. doi: 10.1016/j.neuroimage.2018.06.018. URL https://pubmed.ncbi.nlm.nih.gov/29890325/.

Michael M. Bronstein, Joan Bruna, Yann LeCun, Arthur Szlam, and Pierre Vandergheynst. Geometric deep learning: going beyond euclidean data. CoRR, abs/1611.08097, 2016. URL http://arxiv.org/abs/1611.08097.

Michael M. Bronstein, Joan Bruna, Taco Cohen, and Petar Velickovic. Geometric deep learning: Grids, groups, graphs, geodesics, and gauges. CoRR, abs/2104.13478, 2021. URL https://arxiv.org/abs/2104.13478.
Joan Bruna, Wojciech Zaremba, Arthur Szlam, and Yann LeCun. Spectral networks and locally connected networks on graphs. *2nd International Conference on Learning Representations, ICLR 2014 - Conference Track Proceedings*, 12 2013. URL https://arxiv.org/abs/1312.6203v3.

Jieneng Chen, Yongyi Lu, Qihang Yu, Xiangde Luo, Ehsan Adeli, Yan Wang, Le Lu, Alan L. Yuille, and Yuyin Zhou. Transunet: Transformers make strong encoders for medical image segmentation, 2021a.

Junyu Chen, Yufan He, Eric C. Frey, Ye Li, and Yong Du. Vit-v-net: Vision transformer for unsupervised volumetric medical image registration, 2021b.

Judit Ciarrusta, Ralica Dimitrova, Dafnis Batalle, Jonathan O Muirheartaigh, Lucilio Cordero-Grande, Anthony Price, Emer Hughes, Johanna Kangas, Emily Perry, Ayesha Javed, Jill Demilew, Joseph Hajnal, Anthony David Edwards, Declan Murphy, Tomoki Arichi, and Grainne McAlonan. Emerging functional connectivity differences in newborn infants vulnerable to autism spectrum disorders. *Translational Psychiatry* 2020 10:1, 10: 1–10, 5 2020. ISSN 2158-3188. doi: 10.1038/s41398-020-0805-y. URL https://www.nature.com/articles/s41398-020-0805-y.

Taco S. Cohen, Mario Geiger, Jonas Koehler, and Max Welling. Spherical cnns, 2018.

Lucilio Cordero-Grande, Emer J. Hughes, Jana Hutter, Anthony N. Price, and Joseph V. Hajnal. Three-dimensional motion corrected sensitivity encoding reconstruction for multi-shot multi-slice MRI: Application to neonatal brain imaging. *Magnetic resonance in medicine*, 79(3):1365–1376, mar 2018. ISSN 1522-2594. doi: 10.1002/MRM.26796. URL https://pubmed.ncbi.nlm.nih.gov/28626962/.

Stéphane d’Ascoli, Hugo Touvron, Matthew Leavitt, Ari Morcos, Giulio Biroli, and Levent Sagun. Convit: Improving vision transformers with soft convolutional inductive biases, 2021.

Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional neural networks on graphs with fast localized spectral filtering, 2017.

Michaël Defferrard, Martino Milani, Frédéric Gusset, and Nathanaël Perraudin. Deepsphere: a graph-based spherical cnn, 2020.

Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding, 2019.

Valentina Doria, Christian F. Beckmann, Tomoki Arichi, Nazakat Merchant, Michela Groppo, Federico E. Turkheimer, Serena J. Counsell, Maria Murgasova, Paul Aljabar, Rita G. Nunes, David J. Larkman, Geraint Rees, and A. David Edwards. Emergence of resting state networks in the preterm human brain. *Proceedings of the National Academy of Sciences*, 107(46):20015–20020, 2010. ISSN 0027-8424. doi: 10.1073/pnas.1007921107. URL https://www.pnas.org/content/107/46/20015.
Alexey Dosovitskiy, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, Jakob Uszkoreit, and Neil Houlsby. An image is worth 16x16 words: Transformers for image recognition at scale. *CoRR*, abs/2010.11929, 2020. URL https://arxiv.org/abs/2010.11929.

J. Dubois, M. Benders, A. Cachia, F. Lazeyras, R. Ha-Vinh Leuchter, S. V. Sizonenko, C. Borradori-Tolsa, J. F. Mangin, and P. S. Hüppi. Mapping the early cortical folding process in the preterm newborn brain. *Cerebral cortex (New York, N.Y. : 1991)*, 18:1444–1454, 6 2008. ISSN 1460-2199. doi: 10.1093/CERCOR/BHM180. URL https://pubmed.ncbi.nlm.nih.gov/17934189/.

Vijay Prakash Dwivedi and Xavier Bresson. A generalization of transformer networks to graphs, 2021.

Michael Eyre, Sean P. Fitzgibbon, Judit Ciarrusta, Lucilio Cordero-Grande, Anthony N. Price, Tanya Poppe, Andreas Schul, Emer Hughes, Camilla O’Keeffe, Jakki Brandon, Daniel Cromb, Katy Vecchiato, Jesper Andersson, Eugene P. Duff, Serena J. Counsell, Stephen M. Smith, Daniel Rueckert, Joseph V. Hajnal, Tomoki Arichi, Jonathan O’Muircheartaigh, Dafnis Batalle, and A. David Edwards. The developing human connectome project: typical and disrupted perinatal functional connectivity. *Brain : a journal of neurology*, 144:2199–2213, 7 2021. ISSN 1460-2156. doi: 10.1093/BRAIN/AWAB118. URL https://pubmed.ncbi.nlm.nih.gov/33734321/.

Abdulah Fawaz, Logan Z. J. Williams, Amir Alansary, Cher Bass, Karthik Gopinath, Mariana da Silva, Simon Dahan, Chris Adamson, Bonnie Alexander, Deanne Thompson, Gareth Ball, Christian Desrosiers, Hervé Lombar, Daniel Rueckert, A. David Edwards, and Emma C. Robinson. Benchmarking geometric deep learning for cortical segmentation and neurodevelopmental phenotype prediction. *bioRxiv*, 2021. doi: 10.1101/2021.12.01.470730. URL https://www.biorxiv.org/content/early/2021/12/02/2021.12.01.470730.

Chun-Mei Feng, Yunlu Yan, Huazhu Fu, Li Chen, and Yong Xu. Task transformer network for joint mri reconstruction and super-resolution, 2021.

Bruce Fischl, Niranjini Rajendra, Evelina Busa, Jean Augustinack, Oliver Hinds, B. T. Thomas Yeo, Hartmut Mohlberg, Katrin Amunts, and Karl Zilles. Cortical folding patterns and predicting cytoarchitecture. *Cerebral cortex (New York, N.Y. : 1991)*, 18(8):1973–1980, aug 2008. ISSN 1460-2199. doi: 10.1093/CERCOR/BHM225. URL https://pubmed.ncbi.nlm.nih.gov/18079129/.

Martin A. Frost and Rainer Goebel. Measuring structural-functional correspondence: spatial variability of specialised brain regions after macro-anatomical alignment. *NeuroImage*, 59(2):1369–1381, jan 2012. ISSN 1095-9572. doi: 10.1016/J.NEUROIMAGE.2011.08.035. URL https://pubmed.ncbi.nlm.nih.gov/21875671/.

Yunhe Gao, Mu Zhou, and Dimitris Metaxas. Utnet: A hybrid transformer architecture for medical image segmentation, 2021.
Matthew F Glasser and David C Van Essen. Mapping human cortical areas in vivo based on myelin content as revealed by t1-and t2-weighted mri. *Journal of Neuroscience*, 31 (32):11597–11616, 2011.

Matthew F. Glasser, Timothy S. Coalson, Emma C. Robinson, Carl D. Hacker, John Harwell, Essa Yacoub, Kamil Ugurbil, Jesper Andersson, Christian F. Beckmann, Mark Jenkinson, Stephen M. Smith, and David C. Van Essen. A multi-modal parcellation of human cerebral cortex. *Nature*, 536(7615):171–178, aug 2016. ISSN 14764687. doi: 10.1038/nature18933. URL https://www.nature.com/articles/nature18933.

Karthik Gopinath, Christian Desrosiers, and Herve Lombaert. Learnable pooling in graph convolution networks for brain surface analysis, 2019.

Meng-Hao Guo, Jun-Xiong Cai, Zheng-Ning Liu, Tai-Jiang Mu, Ralph R. Martin, and Shi-Min Hu. Pct: Point cloud transformer. *Computational Visual Media*, 7(2):187–199, Apr 2021. ISSN 2096-0662. doi: 10.1007/s41095-021-0229-5. URL http://dx.doi.org/10.1007/s41095-021-0229-5.

Lingshen He, Yiming Dong, Yisen Wang, Dacheng Tao, and Zhouchen Lin. Gauge equivariant transformer. In *Thirty-Fifth Conference on Neural Information Processing Systems*, 2021. URL https://openreview.net/forum?id=fyL9HD-kImm.

Jie Hu, Li Shen, Samuel Albanie, Gang Sun, and Enhua Wu. Squeeze-and-excitation networks, 2019.

Emer J. Hughes, Tobias Winchman, Francesco Padorno, Rui Teixeira, Julia Wurie, Maryanne Sharma, Matthew Fox, Jana Hutter, Lucilio Cordero-Grande, Anthony N. Price, Joanna Allsop, Jose Bueno-Conde, Nora Tusor, Tomoki Arichi, A. D. Edwards, Mary A. Rutherford, Serena J. Counsell, and Joseph V. Hajnal. A dedicated neonatal brain imaging system. *Magnetic resonance in medicine*, 78(2):794–804, aug 2017. ISSN 1522-2594. doi: 10.1002/MRM.26462. URL https://pubmed.ncbi.nlm.nih.gov/27643791/.

Max Jaderberg, Karen Simonyan, Andrew Zisserman, and Koray Kavukcuoglu. Spatial transformer networks, 2016.

Chiyu "Max" Jiang, Jingwei Huang, Karthik Kashinath, Prabhat, Philip Marcus, and Matthias Niessner. Spherical cnns on unstructured grids, 2019.

Davood Karimi, Serge Vasylechko, and Ali Gholipour. Convolution-free medical image segmentation using transformers, 2021.

Byung-Hoon Kim, Jong Chul Ye, and Jae-Jin Kim. Learning dynamic graph representation of brain connectome with spatio-temporal attention, 2021.

Thomas N. Kipf and Max Welling. Semi-supervised classification with graph convolutional networks, 2017.
Alexander Kolesnikov, Lucas Beyer, Xiaohua Zhai, Joan Puigcerver, Jessica Yung, Sylvain Gelly, and Neil Houlsby. Large scale learning of general visual representations for transfer. *CoRR*, abs/1912.11370, 2019. URL [http://arxiv.org/abs/1912.11370](http://arxiv.org/abs/1912.11370).

Fanwei Kong and Shawn C. Shadden. Whole heart mesh generation for image-based computational simulations by learning free-from deformations, 2021.

Ru Kong, Jingwei Li, Csaba Orban, Mert R. Sabuncu, Hesheng Liu, Alexander Schaefer, Nanbo Sun, Xi Nian Zuo, Avram J. Holmes, Simon B. Eickhoff, and B. T. Thomas Yeo. Spatial topography of individual-specific cortical networks predicts human cognition, personality, and emotion. *Cerebral cortex (New York, N.Y. : 1991)*, 29:2533–2551, 6 2019. ISSN 1460-2199. doi: 10.1093/CERCOR/BHY123. URL [https://pubmed.ncbi.nlm.nih.gov/29878084/](https://pubmed.ncbi.nlm.nih.gov/29878084/).

Maria Kuklisova-Murgasova, Gerardine Quaghebeur, Mary A. Rutherford, Joseph V. Hajnal, and Julia A. Schnabel. Reconstruction of fetal brain MRI with intensity matching and complete outlier removal. *Medical image analysis*, 16(8):1550–1564, 2012. ISSN 1361-8423. doi: 10.1016/J.MEDIA.2012.07.004. URL [https://pubmed.ncbi.nlm.nih.gov/22939612/](https://pubmed.ncbi.nlm.nih.gov/22939612/).

Leo Lebrat, Rodrigo Santa Cruz, Frederic de Gournay, Darren Fu, Pierrick Bourgeat, Jurgen Fripp, Clinton Fookes, and Olivier Salvado. Corticalflow: A diffeomorphic mesh transformer network for cortical surface reconstruction. In *Thirty-Fifth Conference on Neural Information Processing Systems*, 2021. URL [https://openreview.net/forum?id=wD6GWHqLuhS](https://openreview.net/forum?id=wD6GWHqLuhS).

Ze Liu, Jia Ning, Yue Cao, Yixuan Wei, Zheng Zhang, Stephen Lin, and Han Hu. Video swin transformer, 2021.

Qiang Ma, Emma C. Robinson, Bernhard Kainz, Daniel Rueckert, and Amir Alansary. Pialnn: A fast deep learning framework for cortical pial surface reconstruction, 2021.

Antonios Makropoulos, Emma C. Robinson, Andreas Schuh, Robert Wright, Sean Fitzgibbon, Jelena Bozek, Serena J. Counsell, Johannes Steinweg, Katy Vecchiato, Jonathan Passerat-Palmbach, Gregor Lenz, Filippo Mortari, Tencho Tenev, Eugene P. Duff, Matteo Bastiani, Lucilio Cordero-Grande, Emer Hughes, Nora Tusor, Jacques Donald Tournier, Jana Hutter, Anthony N. Price, Rui Pedro A.G. Teixeira, Maria Murgasova, Suresh Victor, Christopher Kelly, Mary A. Rutherford, Stephen M. Smith, A. David Edwards, Joseph V. Hajnal, Mark Jenkinson, and Daniel Rueckert. The Developing Human Connectome Project: A Minimal Processing Pipeline for Neonatal Cortical Surface Reconstruction, apr 2018. ISSN 1095-9572. URL [https://pubmed.ncbi.nlm.nih.gov/29409960/](https://pubmed.ncbi.nlm.nih.gov/29409960/).

Federico Monti, Davide Boscaini, Jonathan Masci, Emanuele Rodolà, Jan Svoboda, and Michael M. Bronstein. Geometric deep learning on graphs and manifolds using mixture model cnns, 2016.

Walter Hugo Lopez Pinaya, Petru-Daniel Tudosiu, Robert Gray, Geraint Rees, Parashkev Nachev, Sebastien Ourselin, and M. Jorge Cardoso. Unsupervised brain anomaly detection and segmentation with transformers, 2021.
Alec Radford, Karthik Narasimhan, Tim Salimans, and Ilya Sutskever. Improving language understanding by generative pre-training, 2018. URL https://gluebenchmark.com/leaderboard.

Emma C. Robinson, Saad Jbabdi, Matthew F. Glasser, Jesper Andersson, Gregory C. Burgess, Michael P. Harms, Stephen M. Smith, David C. Van Essen, and Mark Jenkinson. MSM: a new flexible framework for Multimodal Surface Matching. *NeuroImage*, 100:414–426, oct 2014. ISSN 1095-9572. doi: 10.1016/J.NEUROIMAGE.2014.05.069. URL https://pubmed.ncbi.nlm.nih.gov/24939340/.

Emma C. Robinson, Kara Garcia, Matthew F. Glasser, Zhengdao Chen, Timothy S. Coalson, Antonios Makropoulos, Jelena Bozek, Robert Wright, Andreas Schuh, Matthew Webster, Jana Hutter, Anthony Price, Lucilio Cordero Grande, Emer Hughes, Nora Tusor, Philip V. Bayly, David C. Van Essen, Stephen M. Smith, A. David Edwards, Joseph Hajnal, Mark Jenkinson, Ben Glocker, and Daniel Rueckert. Multimodal surface matching with higher-order smoothness constraints. *NeuroImage*, 167:453–465, feb 2018. ISSN 1095-9572. doi: 10.1016/J.NEUROIMAGE.2017.10.037. URL https://pubmed.ncbi.nlm.nih.gov/29100940/.

Ignacio Sarasua, Sebastian Pölsterl, and Christian Wachinger. Transformesh: A transformer network for longitudinal modeling of anatomical meshes. *CoRR*, abs/2109.00532, 2021. URL https://arxiv.org/abs/2109.00532.

Jo Schlemper, Ozan Oktay, Michiel Schaap, Mattias Heinrich, Bernhard Kainz, Ben Glocker, and Daniel Rueckert. Attention gated networks: Learning to leverage salient regions in medical images, 2019.

Andreas Schuh, Antonios Makropoulos, Robert Wright, Emma C. Robinson, Nora Tusor, Johannes Steinweg, Emer Hughes, Lucilio Cordero Grande, Anthony Price, Jana Hutter, Joseph V. Hajnal, and Daniel Rueckert. A deformable model for the reconstruction of the neonatal cortex. *Proceedings - International Symposium on Biomedical Imaging*, pages 800–803, jun 2017. ISSN 19458452. doi: 10.1109/ISBI.2017.7950639.

Jennifer E Soun, Michael Z Liu, Keith A Cauley, and Jack Grinband. Evaluation of neonatal brain myelination using the t1-and t2-weighted mri ratio. *Journal of Magnetic Resonance Imaging*, 46(3):690–696, 2017.

Andreas Steiner, Alexander Kolesnikov, Xiaohua Zhai, Ross Wightman, Jakob Uszkoreit, and Lucas Beyer. How to train your vit? data, augmentation, and regularization in vision transformers. *CoRR*, abs/2106.10270, 2021. URL https://arxiv.org/abs/2106.10270.

Hugo Touvron, Andrea Vedaldi, Matthijs Douze, and Hervé Jégou. Fixing the train-test resolution discrepancy. *CoRR*, abs/1906.06423, 2019. URL http://arxiv.org/abs/1906.06423.

Hugo Touvron, Matthieu Cord, Matthijs Douze, Francisco Massa, Alexandre Sablayrolles, and Hervé Jégou. Training data-efficient image transformers & distillation through attention. *CoRR*, abs/2012.12877, 2020. URL https://arxiv.org/abs/2012.12877.
Gijs van Tulder, Yao Tong, and Elena Marchiori. Multi-view analysis of unregistered medical images using cross-view transformers. *Lecture Notes in Computer Science*, page 104–113, 2021. ISSN 1611-3349. doi: 10.1007/978-3-030-87199-4_10. URL http://dx.doi.org/10.1007/978-3-030-87199-4_10.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. Attention is all you need. *CoRR*, abs/1706.03762, 2017. URL http://arxiv.org/abs/1706.03762.

Xiaolong Wang, Ross Girshick, Abhinav Gupta, and Kaiming He. Non-local neural networks, 2018a.

Xiaosong Wang, Yifan Peng, Le Lu, Zhiyong Lu, and Ronald M. Summers. Tienet: Text-image embedding network for common thorax disease classification and reporting in chest x-rays, 2018b.

Logan Z. J. Williams, Sean P. Fitzgibbon, Jelena Bozek, Anderson M. Winkler, Ralica Dimitrova, Tanya Poppe, Andreas Schuh, Antonios Makropoulos, John Cupitt, Jonathan O’Muircheartaigh, Eugene P. Duff, Lucilio Cordero-Grande, Anthony N. Price, Joseph V. Hajnal, Daniel Rueckert, Stephen M. Smith, A. David Edwards, and Emma C. Robinson. Structural and functional asymmetry of the neonatal cerebral cortex. *bioRxiv*, 2021. doi: 10.1101/2021.10.13.464206. URL https://www.biorxiv.org/content/early/2021/10/13/2021.10.13.464206.

Mengde Xu, Zheng Zhang, Han Hu, Jianfeng Wang, Lijuan Wang, Fangyun Wei, Xiang Bai, and Zicheng Liu. End-to-end semi-supervised object detection with soft teacher, 2021.

Junhan Yang, Zheng Liu, Shitao Xiao, Chaozhuo Li, Defu Lian, Sanjay Agrawal, Amit Singh, Guangzhong Sun, and Xing Xie. Graphformers: Gnn-nested transformers for representation learning on textual graph, 2021.

Yundong Zhang, Huiye Liu, and Qiang Hu. Transfuse: Fusing transformers and cnns for medical image segmentation, 2021a.

Yungeng Zhang, Yuru Pei, and Hongbin Zha. Learning dual transformer network for diffeomorphic registration. In Marleen de Bruijne, Philippe C. Cattin, Stéphane Cotin, Nicolas Padov, Stefanie Speidel, Yefeng Zheng, and Caroline Essert, editors, *Medical Image Computing and Computer Assisted Intervention – MICCAI 2021*, pages 129–138, Cham, 2021b. Springer International Publishing. ISBN 978-3-030-87202-1.

Fenqiang Zhao, Shunren Xia, Zhengwang Wu, Dingna Duan, Li Wang, Weili Lin, John H Gilmore, Dinggang Shen, and Gang Li. Spherical u-net on cortical surfaces: Methods and applications, 2019.

Hengshuang Zhao, Li Jiang, Jiaya Jia, Philip H.S. Torr, and Vladlen Koltun. Point transformer. In *Proceedings of the IEEE/CVF International Conference on Computer Vision (ICCV)*, pages 16259–16268, October 2021.
Appendix A. Training details

A.1. Experimental set-up & training strategy

All experiments were run on a single NVIDIA TITAN RTX or RTX 3090 24GB GPU. The batch size was maximised to use all GPU memory at training time (256 for SiT-Tiny, 128 for SiT-Small and 64 for SiT-Base). The training strategy used for each task and model is summarised in Table 3. For trainings from ImageNet or MPP weights, models were finetuned for 1000 epochs, as their convergence was faster. Models were optimised similarly for native and template space. Linear warm-up was used for 50 epochs. MSE loss is used for optimisation.

| Model     | Task | Optimiser | Warm-up | Learning Rate | Training Iterations |
|-----------|------|-----------|---------|---------------|---------------------|
| SiT-tiny  | PMA  | SGD       | ✓       | 1e−4          | 2000                |
| SiT-tiny  | GA   | Adam      | ✓       | 5e−4          | 2000                |
| SiT-tiny  | GA   | Adam      | ✓       | 5e−4          | 2000                |
| SiT-base  | PMA  | SGD       | ✓       | 1e−5          | 1000                |
| SiT-base  | GA   | Adam      | ✓       | 5e−5          | 1000                |
| SiT-base  | GA   | Adam      | ✓       | 5e−5          | 1000                |
| SiT-base  | GA   | Adam      | ✓       | 5e−5          | 1000                |

Table 3: Training strategies for all models and task. Finetuning refers to models trained from ImageNet weights or after self-supervision (MPP).

A.2. Hyperparameter search & training strategy

A hyperparameter search was run for the PMA and GA (Table 4) prediction tasks. Hyperparameters were optimised for the SiT-tiny model and include choice of optimiser and best learning strategy, where this includes investigating use of a scheduler, and performing warm up. For the task of PMA prediction, the hyperparameter search suggested best use of SGD with warm-up; whereas for GA, best models were obtained using Adam.

A.3. Pre-processing

Surface data used were generated by the dHCP structural pipeline (Makropoulos et al., 2018). Briefly, motion-corrected, reconstructed T2w and T1w images were bias corrected and brain extracted. Next, images were segmented into several tissue types using the Draw-EM algorithm. Following this, topologically correct white matter surfaces were fit to the grey-white tissue boundary. Pial surfaces were then generated by expanding the white matter mesh towards the grey-cerebrospinal fluid boundary. Inflated surfaces (including spheres) were generated through an iterative process of inflation and smoothing. The dHCP structural pipeline generated a number of univariate features surface-based features summarising cortical organisation. In this paper, we used: sulcal depth, curvature, cortical thickness (estimated as the Euclidean distance between corresponding vertices in the white and pial surfaces), and the T1w/T2w ratio maps, which are highly correlated with intracortical myelination (Glasser and Van Essen, 2011; Soun et al., 2017).

Spherical-based surface registration was performed using Multimodal Surface Matching (Robinson et al., 2014, 2018) using sulcal depth as the sole feature. All data were registered.
| Optimiser | Learning Rate | Warm-up | Scheduler | PMA     | GA     |
|-----------|---------------|---------|-----------|---------|--------|
| SGD       | 5e^{-3}       | x       | x         | +∞      | +∞     |
| SGD       | 1e^{-3}       | x       | x         | 0.912   | 1.549  |
| SGD       | 5e^{-4}       | x       | x         | 0.653   | 1.504  |
| SGD       | 1e^{-4}       | x       | x         | 0.680   | 1.586  |
| SGD       | 5e^{-5}       | x       | x         | 0.721   | 1.588  |
| Adam      | 5e^{-3}       | x       | x         | 0.684   | 1.663  |
| Adam      | 1e^{-3}       | x       | x         | 1.005   | 1.684  |
| Adam      | 5e^{-4}       | x       | x         | 0.918   | 1.372  |
| Adam      | 1e^{-4}       | x       | x         | 0.766   | 2.244  |
| Adam      | 5e^{-5}       | x       | x         | 1.381   | 26.76  |
| SGD       | 5e^{-4}       | ✔️50    | x         | 0.641   | 1.481  |
| SGD       | 5e^{-4}       | ✔️50    | x         | 0.714   | -      |
| SGD       | 5e^{-4}       | ✔️100   | x         | 0.643   | -      |
| SGD       | 5e^{-4}       | ✔️50    | Cosine    | 0.645   | -      |
| Adam      | 5e^{-3}       | ✔️50    | x         | 0.844   | 1.518  |
| Adam      | 5e^{-3}       | ✔️50    | Cosine    | 0.973   | -      |
| Adam      | 5e^{-4}       | ✔️50    | x         | -       | 1.437  |

Table 4: Optimising strategy and hyperparameter search for PMA and GA (template aligned data). Mean Absolute Error (MAE) in weeks on the validation set. Models were trained for 1000 iterations.

to a modified version of the 40-week sulcal depth template from the dHCP spatiotemporal cortical surface atlas (Bozek et al., 2018), which was made to be left-right symmetric (Williams et al., 2021). In this paper, template space refers to sphericalised cortical surface data registered to the 40-week template, and native space refers to sphericalised cortical surface data prior to registration. Finally, the cortical data is resampled, using barycentric interpolation, from its template resolution (32492 vertices) to a sixth order icosphere (mesh of 40962 equally spaced vertices).

In all experiments, datasets were group-normalised across feature channels to a mean of 0 and standard deviation of 1, and split into train/validation/test ratio: 80%/10%/10%.

A.4. Training of gDL methods

The proposed vision transformer framework is benchmarked against five geometric deep learning methods for estimating surface convolutions, including two graph convolutional networks: ChebNet (Defferrard et al., 2017) and GConvNet (Kipf and Welling, 2017); S2CNN (Cohen et al., 2018) - which implements spectral convolutions in $S^0(3)$; Spherical-Unet (Zhao et al., 2019), which learns localised filters fit to the hexagonal tessellation of a regular icosphere; and MoNet (Monti et al., 2016), which fits filters as a mixture of isotropic and anisotropic Gaussians. All networks were implemented with 4 convolutional layers, each followed by a ReLU activation and a downsampling operation. Channel size doubled after each convolution from an initial value that was set to 32, for all models except S2CNN which began at 16 due to memory constraints. A fully connected layer was used to make a final age prediction, where for birth age prediction, an additional 1D convolution was used to incorporate scan age as a confound. Data augmentation was implemented with
rotations of the icospheres and non-linear warpings of the icosahedral meshes. Balancing of the datasets between terms and preterms was also implemented. For more details see Fawaz et al. 2021.

Appendix B. Additional Results

B.1. Self-Supervision

Various settings for the self-supervision task of masked patch prediction (MPP) have been tested and then finetuned for the task of PMA. In Table 5, we report results with and without finetuning the entire model but only the MLP head. Pretraining is evaluated with template data only or both template and native data; and with a probability of masking patches in the sequence of either 25% or 50%. In either configuration, pretrained models are then finetuned with only the MLP head trainable (✓) or all layers (✓). The baseline corresponds to a pretraining task on template data with 50% chance of masking patches in the sequence with only the MLP head finetuned for the PMA task (first row in Table 5).

Table 5: Masked patch prediction task. Models are trained for 1000 iterations, finetuning on the task of PMA on template data - results are presented on validation set.

| Models     | Pretraining | Template | Native | Prob.Mask. | Finetuning | Params. | PMA    | ∆     |
|------------|-------------|----------|--------|------------|------------|---------|--------|-------|
| SiT-tiny   | dHCP        | ✓        | ❌      | 0.5        | ✓          | 577     | 0.691  | base. |
| SiT-tiny   | dHCP        | ✓        | ❌      | 0.5        | ✓          | 5M      | 0.597  | -13.6%|
| SiT-tiny   | dHCP        | ✓        | ❌      | 0.25       | ✓          | 577     | 0.851  | +23.2 |
| SiT-tiny   | dHCP        | ✓        | ❌      | 0.25       | ✓          | 5M      | 0.817  | +18.2%|
| SiT-tiny   | dHCP        | ✓        | ✓       | 0.5        | ✓          | 577     | 0.710  | +2.7% |
| SiT-tiny   | dHCP        | ✓        | ✓       | 0.5        | ✓          | 5M      | 0.680  | -1.6% |
| SiT-tiny   | ImageNet    | ✓        | ❌      | 0.5        | ✓          | 577     | 0.795  | +15.0%|
| SiT-tiny   | ImageNet    | ✓        | ✓       | 0.5        | ✓          | 5M      | 0.675  | -2.3% |

Table 6: Deconfounding strategy. As explained in Section 4, the scans used for term and preterm subjects for the task of birth age prediction (GA) are confounded by appearance of the scans, and therefore the PMA at scan. Deconfounding PMA at scan for this task constitutes a solution to improve prediction results of birth age. A simple framework for deconfounding the data is illustrated in Figure 3, where the PMA at scan per subject is normalised with a BatchNorm layer and then projected via a learnable linear layer to a vector of dimension $D$. The resulting embedding is added to the sequence of patch embeddings. In Table 6, results before and after deconfounding are presented with a SiT-tiny model for both template and native data.

Appendix C. Vision Surface Transformers

C.1. Multi-Head Self-Attention

Self-attention is the main operation (Eq.2) of the MSA layers. Implemented as:

$$\text{Attention}(Q, K, V) = \text{Softmax} \left( \frac{QK^\top}{\sqrt{D}} \right) V$$

(2)
Methods | Pretraining - MPP | GA Native | GA Template
--- | --- | --- | ---
SiT-tiny | × | 1.85 | 1.38
SiT-tiny | ✓ | 1.76 | 1.25
SiT-tiny-deconfounded | × | 1.66 | 1.37
SiT-tiny-deconfounded | ✓ | 1.61 | 1.18

Table 6: Best results on birth age (GA) prediction task, with and without deconfounding strategy. Comparison with SiT-tiny models trained from scratch and after pretraining.

Figure 3: Illustration of the Surface Vision Transformer model implementation a deconfounding strategy of PMA for the GA prediction task.

it is based on the computation of attention weights between tokens in a sequence. Here, each element of the input sequence is associated with a triplet: the Query, Key, and Value ($Q, K, V \in \mathbb{R}^{N \times D}$) with each computed via linear projection of the input tokens (see Figure 4.a), such that: $Q = XW_Q$, $V = XW_V$, $K = XW_K$. From these, self-attention weights ($\omega_i = [\omega_{i,j}]_{j=1...N}$) are estimated for each patch $i$, from the inner product $\omega_{i,j} = \langle q_i, k_j \rangle$, between the query ($q_i$) of patch $i$, and keys from all patches ($k_j, \forall j \in [1, N]$). From this the self-attention matrix $A = \text{Softmax} \left( \frac{QK^\top}{\sqrt{D}} \right) \in \mathbb{R}^{N \times N}$ is then constructed; normalised (Figure 4.b) and passed through a softmax layer (per row) (Figure 4.c). Finally the output sequence is obtained by weighting the values columns $V$ based on the self-attention weights (Figure 4.d).

C.2. Positional Embeddings

A positional embedding vector $E \in \mathbb{R}^D$ is added to each patch embedding of the sequence $X^{(0)}$. This vector should encode spatial information about the sequence of patches. The
SiT implements a positional encoding in the form of a 1D learnable weights, similar to the approach employed in Dosovitskiy et al. 2020.

C.3. Attention maps

Additional illustrations of attention maps are provided in Figure 5 and Figure 6. Template maps for term and preterm per attention head were created by averaging all attention maps for term and preterm subjects. Attention maps are generated from models trained for the PMA task from scratch Figure 5.a and after self-supervision Figure 5.b, and similarly for the task of GA in Figure 6. Those templates provide valuable insights on both prediction tasks and subjects (see legends in Figure 5 and 6).
Figure 5: Average attention maps in the PMA prediction task across heads for term and preterm neonates (a) when training from scratch and (b) training after self-supervision. With self-supervision, attention shifts away from the medial wall cut (an artefact of cortical surface processing), towards the lateral cortical surface. Attention is complementary across heads, and is highest in association cortical areas, which is consistent with the primary-to-association trajectory of cortical development in the perinatal period. Moreover, attention maps are similar between preterm and term neonates.

Figure 6: Average attention maps in the GA prediction task across heads for term and preterm neonates (a) when training from scratch and (b) training after self-supervision. Unlike the PMA task, the medial wall cut remains an important feature even in models trained with self-supervision which may be due to the fact that predicting GA is a harder task. Areas of high attention are less common in these average maps, and may reflect that cortical areas important for GA prediction are more variable across subjects.
